



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 12:24 PM UTC

PDB ID : 2XHV / pdb_00002xhv
Title : HCV-J4 NS5B Polymerase Point Mutant Orthorhombic Crystal Form
Authors : Harrus, D.; Ahmed-El-Sayed, N.; Simister, P.C.; Miller, S.; Triconnet, M.;
Hagedorn, C.H.; Mahias, K.; Rey, F.A.; Astier-Gin, T.; Bressanelli, S.
Deposited on : 2010-06-21
Resolution : 1.90 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

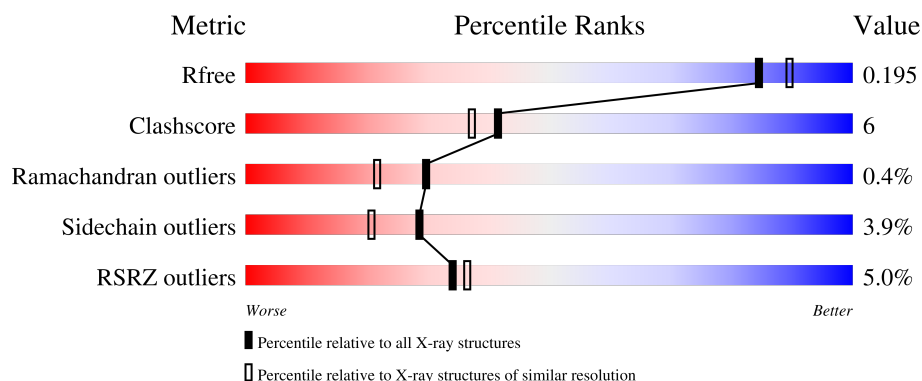
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

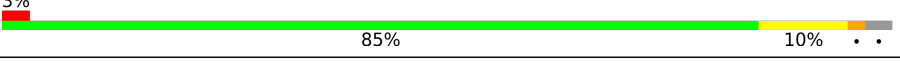
The reported resolution of this entry is 1.90 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	579	
1	B	579	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 9656 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called RNA-directed RNA polymerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	563	Total	C	N	O	S	0	3	0
			4402	2772	777	821	32			
1	B	563	Total	C	N	O	S	0	8	0
			4430	2793	783	821	33			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	ALA	-	expression tag	UNP O92972
A	556	LYS	SER	engineered mutation	UNP O92972
A	571	LEU	-	expression tag	UNP O92972
A	572	GLU	-	expression tag	UNP O92972
A	573	HIS	-	expression tag	UNP O92972
A	574	HIS	-	expression tag	UNP O92972
A	575	HIS	-	expression tag	UNP O92972
A	576	HIS	-	expression tag	UNP O92972
A	577	HIS	-	expression tag	UNP O92972
A	578	HIS	-	expression tag	UNP O92972
B	0	ALA	-	expression tag	UNP O92972
B	556	LYS	SER	engineered mutation	UNP O92972
B	571	LEU	-	expression tag	UNP O92972
B	572	GLU	-	expression tag	UNP O92972
B	573	HIS	-	expression tag	UNP O92972
B	574	HIS	-	expression tag	UNP O92972
B	575	HIS	-	expression tag	UNP O92972
B	576	HIS	-	expression tag	UNP O92972
B	577	HIS	-	expression tag	UNP O92972
B	578	HIS	-	expression tag	UNP O92972

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	1
			10	8	2		
2	A	1	Total	O	S	0	1
			20	16	4		
2	A	1	Total	O	S	0	1
			10	8	2		
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	1
			10	8	2		
2	B	1	Total	O	S	0	1
			20	16	4		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Mg	0	0
			1	1		
3	B	1	Total	Mg	0	0
			1	1		

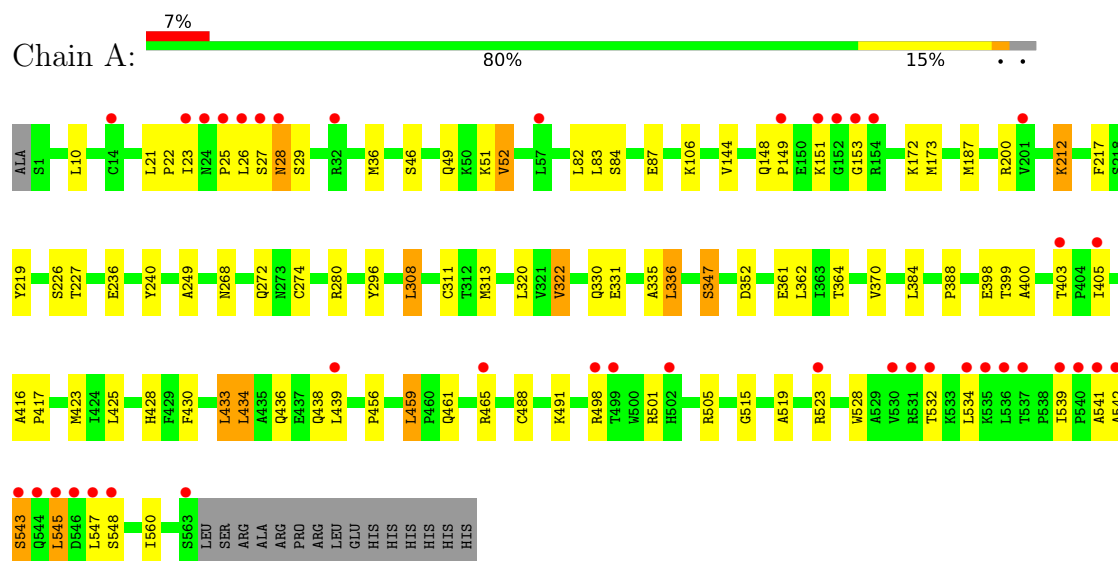
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	278	Total	O	0	0
			278	278		
4	B	409	Total	O	0	0
			409	409		

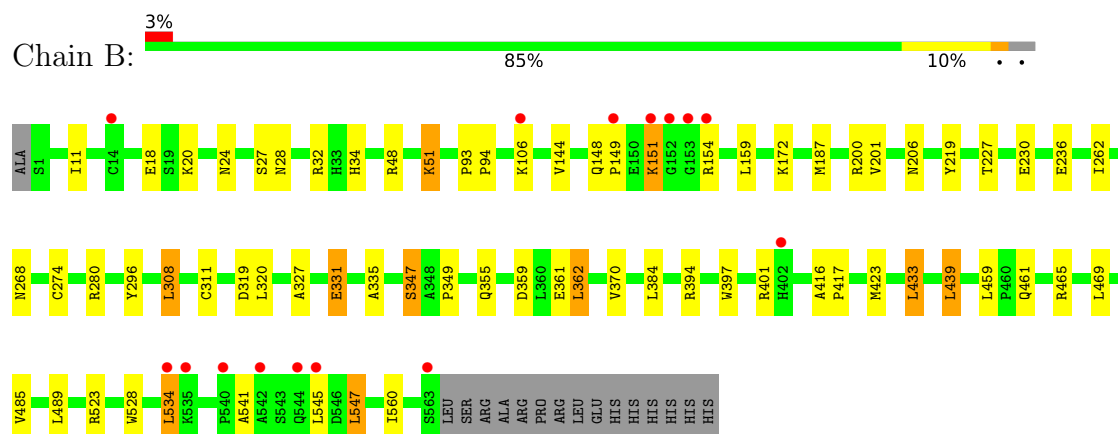
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: RNA-directed RNA polymerase



• Molecule 1: RNA-directed RNA polymerase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	105.74Å 107.69Å 133.84Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	34.67 – 1.90 34.67 – 1.90	Depositor EDS
% Data completeness (in resolution range)	98.5 (34.67-1.90) 98.5 (34.67-1.90)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.05 (at 1.89Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.171 , 0.200 0.168 , 0.195	Depositor DCC
R_{free} test set	5945 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	27.4	Xtriage
Anisotropy	0.475	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 46.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.015 for k,h,-l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	9656	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.10% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, MG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.41	0/4504	0.71	1/6111 (0.0%)
1	B	0.45	0/4547	0.70	0/6168
All	All	0.43	0/9051	0.71	1/12279 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	28	ASN	N-CA-C	-5.51	106.25	112.87

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4402	0	4420	66	0
1	B	4430	0	4471	50	0
2	A	65	0	0	1	0
2	B	70	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	278	0	0	1	0
4	B	409	0	0	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	9656	0	8891	115	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (115) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:52:VAL:HG22	1:A:226:SER:OG	1.64	0.96
1:B:187:MET:SD	4:B:2177:HOH:O	2.30	0.88
1:A:268:ASN:HD21	1:A:272:GLN:HE21	1.23	0.85
1:B:28:ASN:O	1:B:32[B]:ARG:HD2	1.79	0.83
1:A:398:GLU:HG2	1:A:403:THR:HG21	1.59	0.82
1:B:201:VAL:HG22	1:B:384:LEU:HG	1.62	0.81
1:B:230:GLU:HB3	1:B:262[B]:ILE:HD11	1.67	0.74
1:B:201:VAL:CG2	1:B:384:LEU:HG	2.20	0.71
1:B:308:LEU:HB3	1:B:311:CYS:SG	2.34	0.68
1:B:230:GLU:HG2	1:B:262[B]:ILE:HG12	1.76	0.67
1:A:200:ARG:HD3	1:A:384:LEU:HD11	1.76	0.66
1:B:545:LEU:HG	1:B:547:LEU:HD13	1.77	0.66
1:A:465:ARG:HH11	1:A:545:LEU:HD12	1.60	0.65
1:A:498:ARG:HD3	1:B:206:ASN:HD21	1.63	0.64
1:A:27:SER:HB2	1:A:399:THR:HG21	1.81	0.63
1:A:27:SER:CB	1:A:399:THR:HG21	2.29	0.62
1:B:154:ARG:HD3	4:B:2158:HOH:O	2.00	0.62
1:A:542:ALA:O	1:A:543:SER:HB3	2.00	0.61
1:B:148:GLN:HG3	1:B:149:PRO:HD2	1.82	0.60
1:A:465:ARG:NH1	1:A:545:LEU:HD12	2.16	0.60
1:A:461:GLN:HG2	1:A:541:ALA:HB3	1.82	0.59
1:A:82:LEU:HD13	1:A:249:ALA:HB2	1.84	0.58
1:A:236[A]:GLU:OE2	1:A:280:ARG:NH2	2.34	0.57
1:A:25:PRO:HG2	1:A:28:ASN:HB2	1.86	0.57
1:A:361:GLU:HG3	1:A:370:VAL:O	2.04	0.57
1:A:308:LEU:HB3	1:A:311:CYS:SG	2.45	0.56
1:A:542:ALA:O	1:A:543:SER:CB	2.53	0.56
1:B:200:ARG:HD3	1:B:384:LEU:HD11	1.87	0.56
1:A:465:ARG:HD3	1:A:545:LEU:HD11	1.88	0.56
1:A:519:ALA:O	1:A:523:ARG:HG3	2.05	0.56
1:A:172:LYS:HE3	1:A:560:ILE:HD13	1.89	0.55
1:A:515:GLY:HA2	1:A:519:ALA:HB2	1.89	0.55
1:B:465:ARG:HG3	1:B:545:LEU:HD21	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:187:MET:HE3	1:A:296:TYR:CD1	2.42	0.55
1:B:236[B]:GLU:CD	1:B:280:ARG:HH22	2.15	0.55
1:A:227:THR:HB	1:A:347[B]:SER:O	2.07	0.54
1:B:327:ALA:O	1:B:331:GLU:HG3	2.07	0.54
1:A:36:MET:HE2	1:A:491:LYS:HG2	1.89	0.53
1:B:172:LYS:HE3	1:B:560:ILE:HD13	1.90	0.53
1:A:148:GLN:CG	1:A:149:PRO:HD2	2.38	0.53
1:B:308:LEU:HD13	1:B:335:ALA:HB1	1.91	0.53
1:A:268:ASN:HB3	1:A:274:CYS:SG	2.49	0.53
1:B:34:HIS:HD2	4:B:2022:HOH:O	1.91	0.52
1:A:308:LEU:CD1	1:A:335:ALA:HB1	2.39	0.52
1:A:461:GLN:HG2	1:A:541:ALA:CB	2.40	0.52
1:B:359:ASP:HB3	1:B:362:LEU:HD22	1.91	0.51
1:A:399:THR:OG1	1:A:428:HIS:HE1	1.93	0.51
1:A:545:LEU:HD13	1:A:547:LEU:HD13	1.91	0.51
1:B:268:ASN:HB3	1:B:274:CYS:SG	2.50	0.51
1:B:461:GLN:HG2	1:B:541:ALA:HB3	1.91	0.51
1:A:217:PHE:CD1	1:A:336:LEU:HD11	2.46	0.51
1:B:219:TYR:HB3	1:B:320:LEU:HD23	1.93	0.50
1:B:433:LEU:HB3	1:B:439:LEU:CD1	2.42	0.50
1:B:148:GLN:CG	1:B:149:PRO:HD2	2.41	0.50
1:B:331:GLU:H	1:B:331:GLU:CD	2.18	0.50
1:B:523:ARG:HD3	1:B:534:LEU:HD22	1.93	0.50
1:A:268:ASN:HD21	1:A:272:GLN:NE2	2.00	0.50
1:B:227:THR:HB	1:B:347[B]:SER:O	2.11	0.49
1:B:18:GLU:HG3	1:B:401:ARG:NH1	2.26	0.49
1:B:361:GLU:HG3	1:B:370:VAL:O	2.14	0.48
1:A:51:LYS:HE2	4:A:2043:HOH:O	2.13	0.47
1:B:397:TRP:CE2	1:B:401:ARG:HD2	2.49	0.47
1:A:84:SER:OG	1:A:87:GLU:HG3	2.14	0.47
1:B:327:ALA:O	1:B:331:GLU:CG	2.62	0.47
1:B:433:LEU:HB3	1:B:439:LEU:HD13	1.95	0.47
1:A:313:MET:HG2	1:A:322:VAL:HB	1.97	0.47
1:A:532:THR:O	1:A:532:THR:HG23	2.15	0.47
1:A:27:SER:C	1:A:29:SER:N	2.70	0.47
1:A:148:GLN:HG2	1:A:149:PRO:HD2	1.96	0.47
1:A:433:LEU:HD12	1:A:438:GLN:HB2	1.97	0.46
1:B:236[B]:GLU:OE2	1:B:280:ARG:NH2	2.45	0.46
1:B:347[B]:SER:C	1:B:349:PRO:HD3	2.40	0.46
1:A:501:ARG:HE	1:A:505:ARG:NH2	2.14	0.46
1:A:416:ALA:N	1:A:417:PRO:HD2	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:83:LEU:HB2	1:A:173:MET:HA	1.97	0.46
1:A:26:LEU:HB3	1:A:400:ALA:HA	1.98	0.45
1:A:26:LEU:HD23	1:A:26:LEU:O	2.16	0.45
1:B:24:ASN:HB3	1:B:27:SER:OG	2.17	0.45
1:A:236[A]:GLU:CD	1:A:280:ARG:HH22	2.23	0.45
1:B:11:ILE:HD13	1:B:159:LEU:HD22	1.98	0.45
1:B:465:ARG:HG3	1:B:545:LEU:CD2	2.47	0.44
1:B:423:MET:HA	1:B:528:TRP:CZ2	2.53	0.44
1:A:456:PRO:HA	1:A:459:LEU:HD22	1.99	0.44
1:A:22:PRO:CG	1:A:400:ALA:HB1	2.48	0.44
1:A:439:LEU:O	1:A:456:PRO:HG2	2.18	0.44
1:A:27:SER:HB3	1:A:399:THR:HG21	1.99	0.44
1:B:144:VAL:HB	1:B:394:ARG:HG2	2.01	0.43
1:A:27:SER:C	1:A:29:SER:H	2.25	0.43
1:B:51:LYS:HE3	1:B:51:LYS:HB2	1.59	0.43
1:A:27:SER:HB2	1:A:399:THR:CG2	2.46	0.43
1:A:217:PHE:CE1	1:A:322:VAL:HG22	2.54	0.42
1:A:388:PRO:HG2	1:A:488:CYS:SG	2.60	0.42
1:B:20:LYS:HD3	1:B:20:LYS:HA	1.82	0.42
1:A:501:ARG:O	1:A:505:ARG:HG3	2.19	0.42
1:B:416:ALA:N	1:B:417:PRO:CD	2.83	0.42
1:B:93:PRO:HA	1:B:94:PRO:HD3	1.91	0.42
1:A:148:GLN:HB3	1:A:153:GLY:HA3	2.02	0.41
1:A:532:THR:HG22	2:A:1571:SO4:S	2.60	0.41
1:B:32[B]:ARG:NH2	4:B:2039:HOH:O	2.53	0.41
1:A:434:LEU:HD12	1:A:434:LEU:HA	1.88	0.41
1:B:48[B]:ARG:HG2	1:B:159:LEU:HG	2.03	0.41
1:A:430:PHE:O	1:A:434:LEU:HB2	2.21	0.41
1:A:465:ARG:HD3	1:A:545:LEU:CD1	2.51	0.41
1:B:151:LYS:HA	1:B:151:LYS:HD3	1.34	0.41
1:B:187:MET:HE3	1:B:296:TYR:CD1	2.56	0.41
1:B:485:VAL:O	1:B:489:LEU:HG	2.20	0.41
1:A:219:TYR:HB3	1:A:320:LEU:HD23	2.03	0.41
1:A:545:LEU:HD12	1:A:545:LEU:H	1.85	0.41
1:A:212:LYS:HB2	1:A:212:LYS:NZ	2.36	0.41
1:A:236[B]:GLU:OE2	1:A:240:TYR:OH	2.32	0.40
1:B:362:LEU:HD12	1:B:362:LEU:HA	1.93	0.40
1:A:46:SER:HA	1:A:49:GLN:HE21	1.86	0.40
1:A:539:ILE:HG22	1:A:541:ALA:H	1.87	0.40
1:A:423:MET:HE3	1:A:528:TRP:CZ3	2.56	0.40
1:B:200:ARG:HD3	1:B:384:LEU:CD1	2.51	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	564/579 (97%)	550 (98%)	9 (2%)	5 (1%)	14	6
1	B	569/579 (98%)	557 (98%)	10 (2%)	2 (0%)	30	22
All	All	1133/1158 (98%)	1107 (98%)	19 (2%)	7 (1%)	30	13

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	543	SER
1	A	347[A]	SER
1	A	347[B]	SER
1	A	548	SER
1	A	151	LYS
1	B	347[A]	SER
1	B	347[B]	SER

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	482/493 (98%)	459 (95%)	23 (5%)	23	15
1	B	487/493 (99%)	473 (97%)	14 (3%)	37	31
All	All	969/986 (98%)	932 (96%)	37 (4%)	28	21

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	LEU
1	A	21	LEU
1	A	23	ILE
1	A	52	VAL
1	A	106	LYS
1	A	144	VAL
1	A	212	LYS
1	A	308	LEU
1	A	322	VAL
1	A	330	GLN
1	A	331	GLU
1	A	336	LEU
1	A	352	ASP
1	A	362	LEU
1	A	364	THR
1	A	405	ILE
1	A	425	LEU
1	A	433	LEU
1	A	434	LEU
1	A	436	GLN
1	A	459	LEU
1	A	534	LEU
1	A	545	LEU
1	B	51	LYS
1	B	106	LYS
1	B	151	LYS
1	B	308	LEU
1	B	319	ASP
1	B	331	GLU
1	B	355	GLN
1	B	362	LEU
1	B	433	LEU
1	B	439	LEU
1	B	459	LEU
1	B	469	LEU
1	B	534	LEU
1	B	547	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	28	ASN
1	A	35	ASN
1	A	49	GLN
1	A	206	ASN
1	A	272	GLN
1	A	273	ASN
1	A	330	GLN
1	A	428	HIS
1	A	483	ASN
1	A	514	GLN
1	B	35	ASN
1	B	148	GLN
1	B	206	ASN
1	B	273	ASN
1	B	402	HIS
1	B	446	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 29 ligands modelled in this entry, 2 are monoatomic - leaving 27 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	SO4	A	1568	-	4,4,4	0.26	0	6,6,6	0.09	0
2	SO4	B	1002[D]	-	4,4,4	0.23	0	6,6,6	0.10	0
2	SO4	B	1002[A]	-	4,4,4	0.24	0	6,6,6	0.09	0
2	SO4	B	1003	-	4,4,4	0.23	0	6,6,6	0.09	0
2	SO4	A	1570	-	4,4,4	0.23	0	6,6,6	0.10	0
2	SO4	A	1567[A]	-	4,4,4	0.26	0	6,6,6	0.14	0
2	SO4	B	1001[A]	-	4,4,4	0.20	0	6,6,6	0.13	0
2	SO4	A	1571	-	4,4,4	0.25	0	6,6,6	0.08	0
2	SO4	A	1002[A]	-	4,4,4	0.23	0	6,6,6	0.07	0
2	SO4	A	1001	-	4,4,4	0.23	0	6,6,6	0.08	0
2	SO4	A	1003[A]	-	4,4,4	0.25	0	6,6,6	0.14	0
2	SO4	B	1002[B]	-	4,4,4	0.23	0	6,6,6	0.13	0
2	SO4	A	1003[D]	-	4,4,4	0.23	0	6,6,6	0.13	0
2	SO4	B	1569	-	4,4,4	0.26	0	6,6,6	0.11	0
2	SO4	B	1568	-	4,4,4	0.23	0	6,6,6	0.23	0
2	SO4	A	1567[B]	-	4,4,4	0.24	0	6,6,6	0.10	0
2	SO4	A	1569	-	4,4,4	0.24	0	6,6,6	0.06	0
2	SO4	B	1001[B]	-	4,4,4	0.22	0	6,6,6	0.09	0
2	SO4	B	1571	-	4,4,4	0.26	0	6,6,6	0.16	0
2	SO4	B	1570	-	4,4,4	0.24	0	6,6,6	0.13	0
2	SO4	A	1002[B]	-	4,4,4	0.23	0	6,6,6	0.11	0
2	SO4	B	1002[C]	-	4,4,4	0.22	0	6,6,6	0.08	0
2	SO4	A	1003[B]	-	4,4,4	0.24	0	6,6,6	0.05	0
2	SO4	B	1572	-	4,4,4	0.24	0	6,6,6	0.11	0
2	SO4	B	1573	-	4,4,4	0.24	0	6,6,6	0.10	0
2	SO4	A	1003[C]	-	4,4,4	0.22	0	6,6,6	0.09	0
2	SO4	B	1567	-	4,4,4	0.24	0	6,6,6	0.09	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1571	SO4	1	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	563/579 (97%)	0.31	41 (7%) 21 22	14, 41, 94, 142	3 (0%)
1	B	563/579 (97%)	-0.07	15 (2%) 56 60	11, 30, 62, 121	8 (1%)
All	All	1126/1158 (97%)	0.12	56 (4%) 34 36	11, 34, 82, 142	11 (0%)

All (56) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	534	LEU	6.7
1	B	152	GLY	6.4
1	A	25	PRO	5.6
1	A	545	LEU	5.4
1	A	26	LEU	5.3
1	B	542	ALA	5.3
1	B	534	LEU	5.3
1	A	27	SER	4.4
1	B	153	GLY	4.4
1	A	405	ILE	4.3
1	B	545	LEU	3.8
1	A	153	GLY	3.7
1	A	152	GLY	3.7
1	A	540	PRO	3.4
1	A	563	SER	3.3
1	A	543	SER	3.3
1	B	151	LYS	3.2
1	A	535	LYS	3.1
1	A	544	GLN	3.1
1	B	540	PRO	3.1
1	A	548	SER	3.0
1	A	151	LYS	2.9
1	A	439	LEU	2.9
1	A	536	LEU	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	498	ARG	2.8
1	A	532	THR	2.8
1	A	149	PRO	2.8
1	A	546	ASP	2.8
1	A	57	LEU	2.7
1	A	547	LEU	2.7
1	A	537	THR	2.6
1	B	563	SER	2.6
1	A	542	ALA	2.6
1	A	23	ILE	2.6
1	A	523	ARG	2.6
1	A	28	ASN	2.6
1	B	402	HIS	2.4
1	B	544	GLN	2.4
1	A	539	ILE	2.3
1	B	149	PRO	2.3
1	A	530	VAL	2.3
1	A	499	THR	2.3
1	A	531	ARG	2.2
1	A	502	HIS	2.2
1	A	403	THR	2.2
1	B	14	CYS	2.2
1	B	106	LYS	2.2
1	A	465	ARG	2.1
1	B	535	LYS	2.1
1	A	541	ALA	2.1
1	B	154	ARG	2.1
1	A	14	CYS	2.1
1	A	201	VAL	2.1
1	A	24	ASN	2.0
1	A	154	ARG	2.0
1	A	32	ARG	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	SO4	A	1571	5/5	0.36	0.17	124,127,127,128	0
2	SO4	A	1570	5/5	0.62	0.14	84,88,92,92	5
2	SO4	B	1567	5/5	0.68	0.13	92,95,97,101	0
2	SO4	B	1003	5/5	0.76	0.15	103,104,106,107	0
2	SO4	B	1571	5/5	0.76	0.14	28,56,59,62	5
2	SO4	A	1569	5/5	0.79	0.10	117,119,122,123	0
2	SO4	B	1573	5/5	0.80	0.16	70,71,75,82	5
2	SO4	A	1003[D]	5/5	0.84	0.19	29,34,39,41	5
2	SO4	A	1003[A]	5/5	0.84	0.19	35,36,43,48	5
2	SO4	B	1570	5/5	0.84	0.12	63,63,68,73	5
2	SO4	A	1003[B]	5/5	0.84	0.19	34,43,48,48	5
2	SO4	B	1572	5/5	0.84	0.20	104,106,109,114	0
2	SO4	A	1003[C]	5/5	0.84	0.19	46,46,47,53	5
3	MG	A	3001	1/1	0.85	0.30	167,167,167,167	0
2	SO4	B	1002[B]	5/5	0.86	0.21	20,38,43,46	5
2	SO4	B	1002[C]	5/5	0.86	0.21	43,45,46,47	5
2	SO4	B	1002[D]	5/5	0.86	0.21	34,36,46,47	5
2	SO4	A	1568	5/5	0.86	0.10	32,48,58,60	5
2	SO4	B	1002[A]	5/5	0.86	0.21	29,34,40,44	5
2	SO4	B	1569	5/5	0.87	0.08	64,64,69,73	0
3	MG	B	3001	1/1	0.87	0.31	57,57,57,57	0
2	SO4	A	1001	5/5	0.88	0.13	60,61,64,68	5
2	SO4	A	1002[B]	5/5	0.89	0.15	36,36,45,48	5
2	SO4	A	1002[A]	5/5	0.89	0.15	53,54,63,63	5
2	SO4	B	1001[B]	5/5	0.92	0.11	34,37,45,45	5
2	SO4	B	1001[A]	5/5	0.92	0.11	35,39,45,45	5
2	SO4	A	1567[B]	5/5	0.93	0.10	74,76,78,81	5
2	SO4	A	1567[A]	5/5	0.93	0.10	33,33,39,41	5
2	SO4	B	1568	5/5	0.97	0.09	42,42,44,55	0

6.5 Other polymers

There are no such residues in this entry.